

Hydrogen combustion in the NPDG cave in ER2

S. Covrig, UNH

April 1, 2006

Introduction

The NPDGamma experiment will operate a 16 liters liquid para-hydrogen target in a steel cave in ER2. The liquid hydrogen is contained in an Al vessel which is isolated from the air in the cave by an Al cryostat. For the duration of the data taking the cryostat is maintained under a vacuum of 10^{-5} torr or better.

A question raised by the Target Safety Review Committee in Nov 2005 was: what will happen if the entire hydrogen escapes and burns inside the cave.

A possible answer is given in what follows.

The simulation

To answer the question posed by the safety committee a simulation was set up in FLUENT 6.2 (www.fluent.com), which is a computational fluid dynamics (CFD) package able to handle cases of combustion. A brief description of the simulation follows, along with the results. In this simulation only the effects in and on the npdg-cave were considered.

The Cave The inside volume of the cave was estimated to be about 66 m^3 . To estimate the volume for air in the cave about 6 m^3 were subtracted from the volume of the cave as being instrumentation. The cave was modeled as a right-angle parallelepiped with sides of $4.6 \times 5.2 \times 2.5$ in meters along x, y, and z respectively. The cave was considered to have steel walls on all sides. The walls were taken to be 0.2 m thick. Thermal conduction in walls was accounted for. The outside shell of the walls was assumed to be adiabatic. The cave walls were considered to be hermetic and rigidly connected. The influence of a vent in the ceiling was also simulated. The air of the cave was assumed of being a mix of only $N_2 : O_2$.

Chemistry The main reaction though which hydrogen is consumed in air is



which means that 1 kg of hydrogen reacts with 8 kg of oxygen to produce 9 kg of water. The reaction has an activation energy of about $3 \cdot 10^7\text{ J/kg}\cdot\text{mol}$. If the activation threshold is reached the chemical reaction is triggered and produces a heat of about $\Delta Q = 285.8\text{ kJ/mol}$. The total amount of hydrogen in the target when the target is full of liquid is about 1.15 kg. The volume of the cave, at the normal Los Alamos atmospheric pressure of about 75.36 kPa, contains about 12 kg of oxygen, which is enough to consume all the hydrogen from the target. In what follows it was neglected the fact that hydrogen is initially in cryogenic conditions and it takes about 1 MJ of heat to bring it to standard conditions, as this is small compared to the total heat from water formation, more than 100 MJ.

Combustion Two general cases were considered in the simulation: a cave with no vent (the most conservative case in estimating the over-pressure inside the cave from hydrogen combustion) and a cave with a vent (in order to mimic a realistic situation a vent of 900 cm^2 area was put in the ceiling at a corner of the cave walls). For the *no-vent* case three hydrogen combustion processes were considered in the simulation. In process 1, hydrogen leaks into the cave from the volume of the cryostat and ignition starts without pre-mixing of hydrogen and air. In process 2, hydrogen leaks into the cave and ignition starts after some pre-mixing occurs (about half of hydrogen pre-mixes with the air in the cave). In process 3, hydrogen

leaks into the cave, completely pre-mixes with air before ignition starts. In all processes, for the case of *no-vent*, conservation of total mass was imposed. For the *vent* case only process 3 was considered. Only four gases were considered in the simulation, N₂, O₂, H₂ and water. The gases were taken to be ideal, their specific heats were corrected for temperature dependence up to 5000 K, but their heat conductivities were considered constant.

The estimate for the over-pressure in the cave is taken to be the ratio of the average pressure in the cave at time t to the initial pressure in the cave, which will be called the pressure factor, pf

$$pf = \frac{p(t)}{p(0)} \quad (2)$$

For the *no-vent* case of hydrogen combustion in the cave the order of magnitude of pf_{max} can be calculated assuming that all the heat from the water formation, eq. 1, is absorbed by the gas-mixture, considered to be ideal, inside the cave,

$$Q = m \cdot c_p \cdot \Delta T \approx 10^8 J \quad (3)$$

where m is the total mass of the gas in the cave and c_p is the specific heat of the gas mixture. From the ideal-gas law

$$\Delta T = \frac{p_i V}{R \nu_i} \cdot \left(\frac{p_f \nu_i}{p_i \nu_f} - 1 \right) \quad (4)$$

$$= T_i \left(\frac{pf_{max} \nu_i}{\nu_f} - 1 \right) \quad (5)$$

$$= \frac{Q}{m c_p} \quad (6)$$

where indices i, f refer to initial-final conditions respectively (final meaning when hydrogen is fully consumed), pf_{max} is the maximum pressure factor, the Greek notation $\nu_{i, f}$ refers to the total number of moles in the respective states and R is the ideal gas universal constant. The maximum pressure factor can be estimated from

$$pf_{max} = \frac{\nu_f}{\nu_i} \cdot \left(1 + \frac{Q}{m c_p T_i} \right) \quad (7)$$

where the initial number of moles is given by the nitrogen and oxygen in the air of the cave and the final number of moles is given by the nitrogen, left-over oxygen and water in the final mixture. Taking the total mass of gasses in the cave to be about 53 kg, the specific heat of the mixture to be that for air in standard conditions, about 1000 J/kg·K, the initial temperature of the air in the cave about 300 K and the ratio of moles about 1.16, the estimate for maximum pressure factor is $pf \approx 8.5$.

Results There are three plots and three image to present the results from the simulation. One plot for the pressure factor, two plots for gas masses, and, two images for temperature profiles in the cave and one image for gas-mixture velocity profile. The summary results are presented in Table 1, where the first three lines are for the *no-vent* case and the last line is for the *vent* case. Δt is the time at which

Table 1: Over-Pressure and Temperature

| Cases | pf_{max} | Δt (s) | $\langle T \rangle_{max}$ (K) | Δt (s) |
|-------------------------|------------|----------------|-------------------------------|----------------|
| H_2 source | 11.3 | 17.8 | 3160 | 13.4 |
| H_2 source and premix | 7.9 | 18.2 | 2414 | 19.7 |
| H_2 premix | 9.5 | 3.2 | 2441 | 3.3 |
| H_2 premix and vent | 5.14 | 0.475 | 2268 | 0.6 |

maximum value was reached from the start of ignition and $\langle T \rangle_{max}$ is the temperature averaged over the volume of the cave.

Comments The evolution of the pressure factor in time is presented in fig. 1, where black is for *no-vent* case with hydrogen sourcing, red is for *no-vent* case with premixing and sourcing, green is for *no-vent* case with pre-mixing and blue is for *vent* case with pre-mixing. For the *no-vent* case if hydrogen is sourced inside during the ignition it seems to lead to long lived combustion processes as the maximum pressure in the cave occurs after about 18 s from the start of the process, while if ignition starts after hydrogen mixes with air, the pre-mixed processes, it seems to lead to short lived combustion, where peak pressure is reached in about 3 s. If the cave has a vent then the combustion process is very fast, similar to a deflagration, as the peak pressure in the cave is reached in less than half a second for the vent size modeled here. The results in Table 1 are consistent with the numerical order of magnitude estimate from eq. 7 for the *no-vent* case.

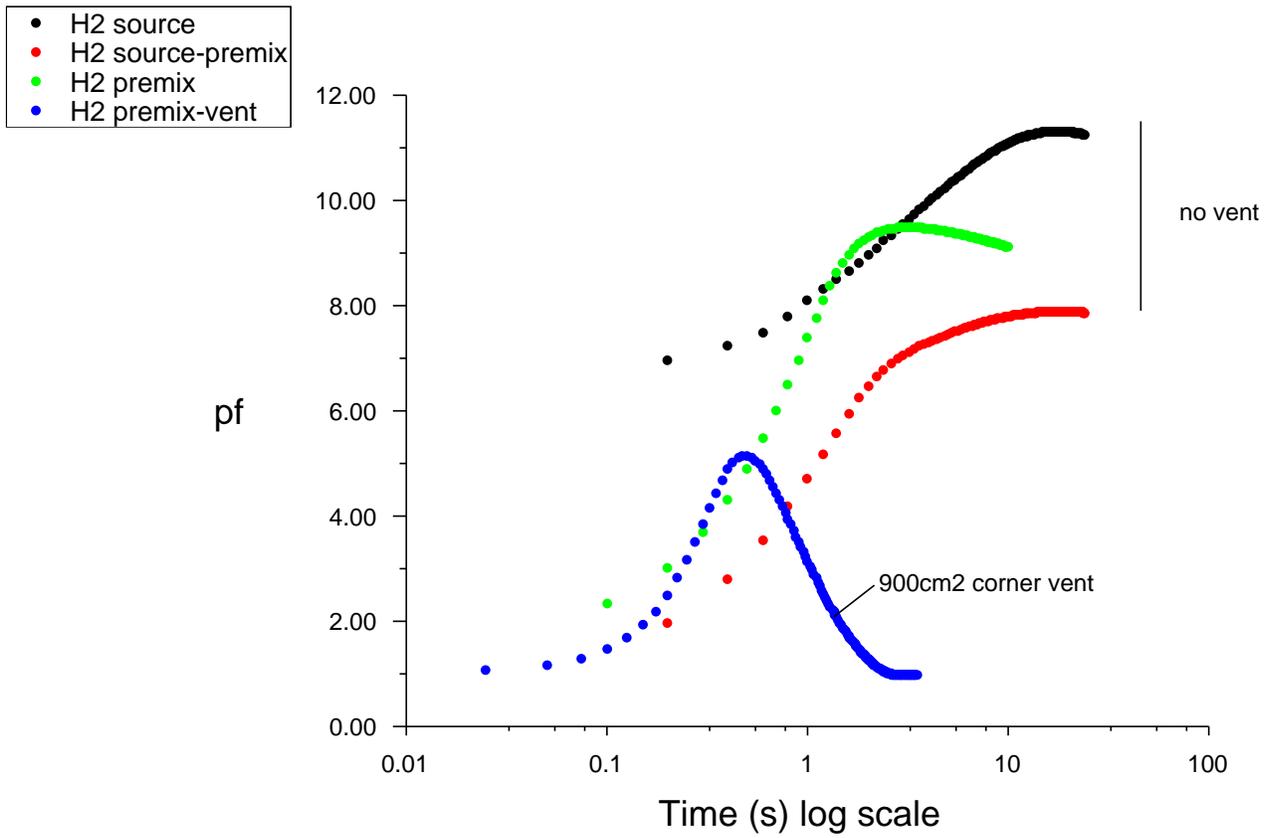
In the *no-vent* case with sourcing the interaction between chemistry and flame was assumed finite-rate-laminar, while in the *no-vent* case with sourcing and pre-mixing and pre-mixing only, stable solutions were reached assuming that the interaction between chemistry and flame is finite-rate-eddy-dissipation.

Fig. 2 shows the behavior of hydrogen and water masses in time, where colors green and blue correspond to *no-vent* case with sourcing, and black and red to *no-vent* case with pre-mixing. Fig. 3 shows the evolution in time of the total gas mass and the hydrogen mass for the *vent* case. In this case as the hydrogen starts burning and the gas-mixture tends to expand it vents through the vent until the total gas-mixture mass reaches a minimum at a time when the heat generated from the water formation is no longer able to sustain the gas expansion and backflow through the vent starts to form, increasing the total mass of the gas-mixture in the cave. The backflow pattern can be seen in fig. 6, which is a snap-shot of contours of constant flow velocity in three sections through the cave and the vent, taken 3.5 s after ignition started.

The images in figs. 4 and 5 show profiles of constant temperature in three sections in the cave for the *no-vent* case with sourcing and pre-mixing, 24 s after ignition started, and, for the *vent* case, 3.5 s after ignition started.

The conditions of the simulation at the cave walls are more stringent than reality. The external shell of the steel walls is in reality in contact with the air in ER2 and so the maximum pressure factor would be expected to be lower in reality than what the simulation calculates. From these results it seems that if hydrogen escapes from the target-cryostat and starts burning in the npdg-cave it can be expected that conditions with pressures of no more than 11 times the local atmospheric pressure and temperatures in excess of 2-3000 K are possible to form inside the cave on time scales of less than 20 s if the cave has no vent. If the cave has a vent similar to the one implemented then an over-pressure of less than half of the worst case scenario for the *no-vent* case could be expected. Another major difference between the *no-vent* and the *vent* cases is the time scale of the combustion, slow and fast (deflagration) respectively.

A few caveats about the CFD engine: a slight dependence of the pf was observed on the size of the mesh elements used to factorize the inside space of the cave, but not significant, the interaction between the turbulence of the flame and the chemistry of combustion has probably the biggest impact on the size and time evolution of pf . A 30% uncertainty can be attributed to turbulence-chemistry interaction effects on pf , which is the difference between the two slow-burning processes, for a *no-vent* case, which were treated with different interactions between chemistry and turbulence of the flame.



Pressure factor

Mar 31, 2006
 FLUENT 6.2 (3d, segregated, lam)

Figure 1: The pressure factor.

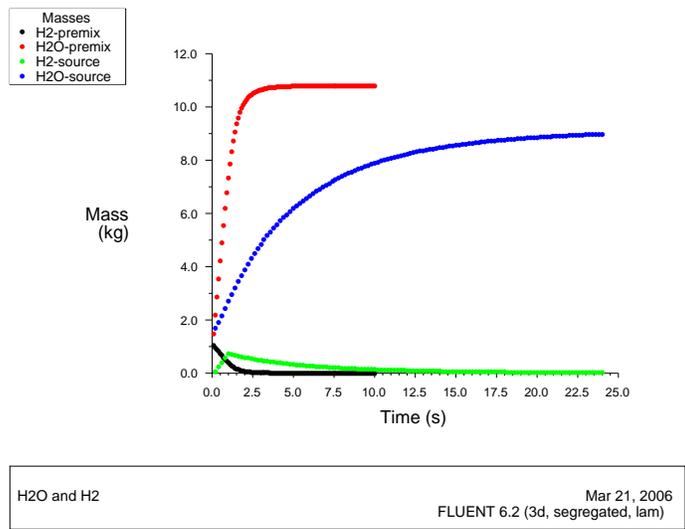


Figure 2: Water production and hydrogen consumption for two processes in the case of *no-vent*

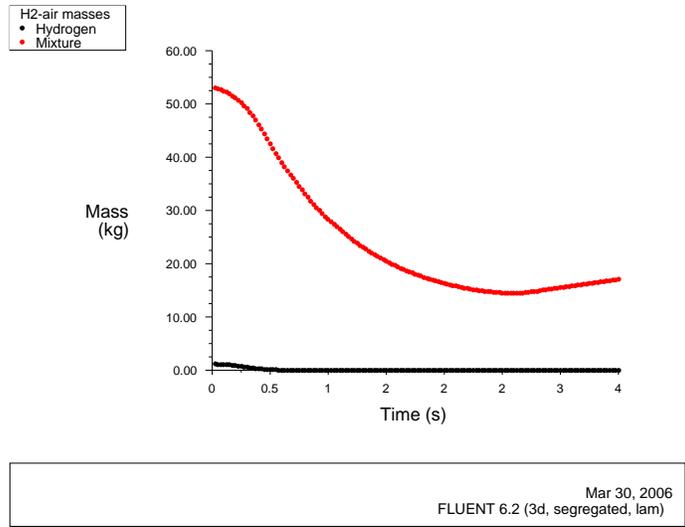


Figure 3: Hydrogen consumption and total gas-mixture mass evolution in the case of *vent*

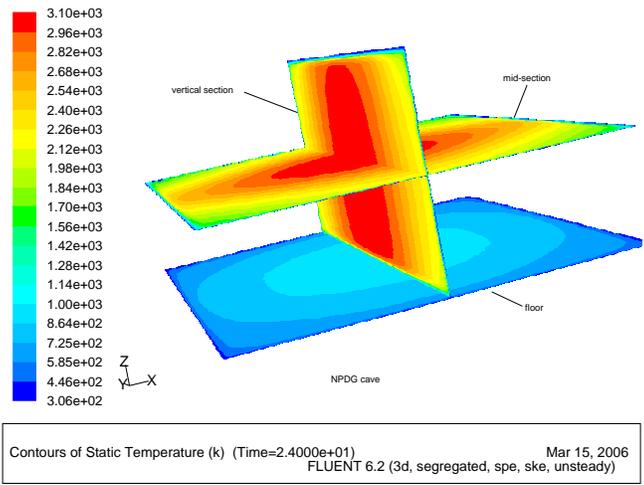


Figure 4: Temperature profile in three sections of the cave with no vent, 24 s after ignition started. Hydrogen premixes before ignition and the walls are adiabatic at the outer shell.

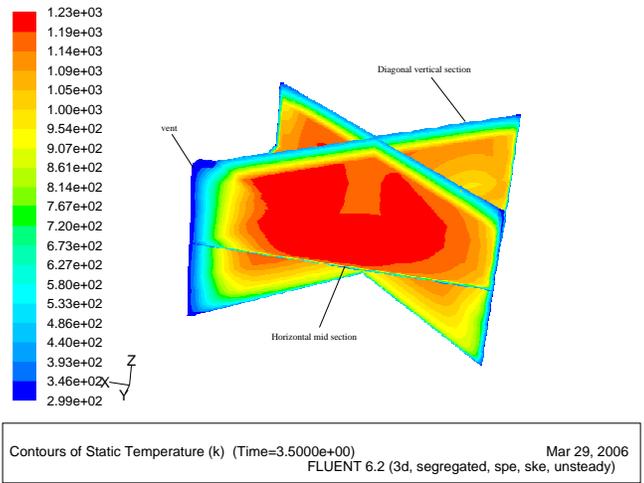
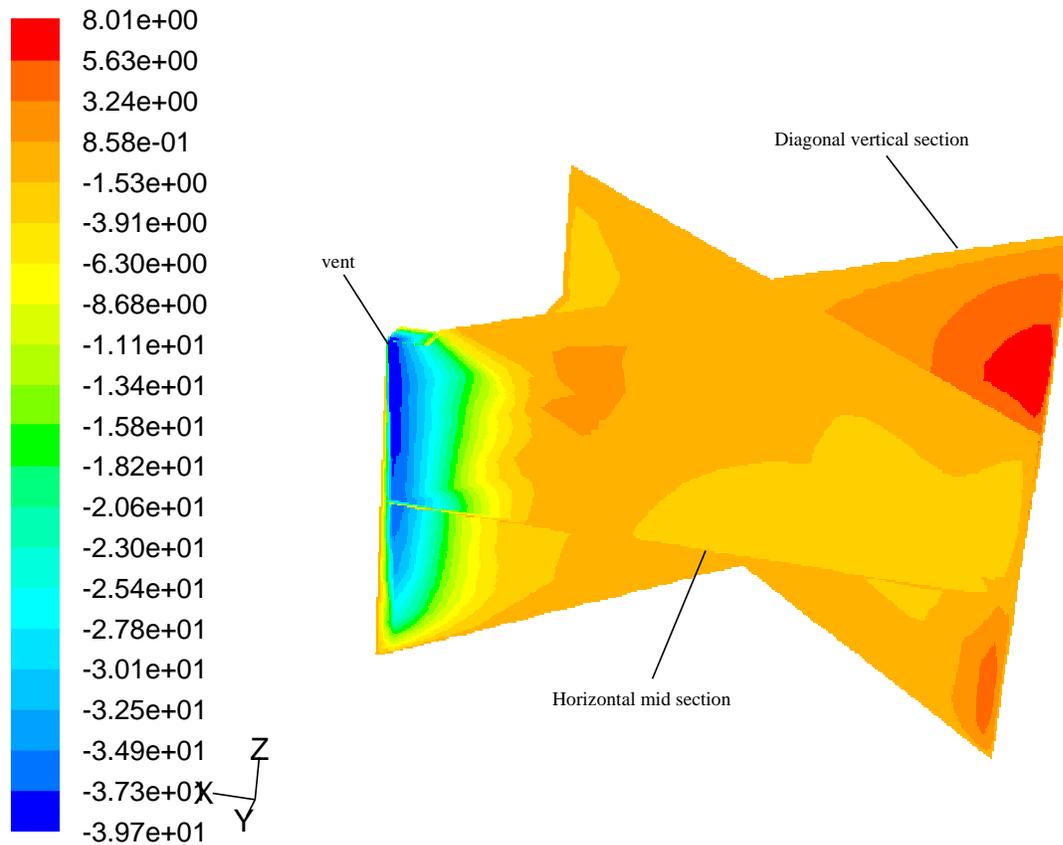


Figure 5: Temperature profile in three sections of the cave 3.5 s after ignition started. Hydrogen premixes before ignition and the cave has a vent 900 cm^2 in a corner in the ceiling wall, the rest of the walls are adiabatic.



Contours of Z Velocity (m/s) (Time=3.5000e+00)

Mar 29, 2006
FLUENT 6.2 (3d, segregated, spe, ske, unsteady)

Figure 6: Flow velocity profile in three sections of the cave 3.5 s after ignition started. Hydrogen premixes before ignition and the cave has a vent 900 cm^2 in a corner in the ceiling wall, the rest of the walls are adiabatic. The air backflows through the vent.